Computational Electromagnetics, Wave Physics, and Quantum Mechanics

Weng Cho CHEW[1]

[1] The University of Hong Kong, Hong Kong SAR, China
Email: wcchew@hku.hk, w-chew@uiuc.edu
(WCC is on leave of absence from the University of Illinois at Urbana Champaign)

Abstract—**In this paper, first, we will discuss the importance of physical insight in computational electromagnetics. We explain why it is relatively easy to arrive at fast algorithms for static problems, but harder for wave physics problems. Second, the understanding of wave physics is very important in classical electromagnetics, but its understanding also allows us to understand other physical phenomena requiring wave physics, such as transport of electrons in complex structures. Last, we discuss the Casimir force calculation that needs a combine understanding of statistical physics, quantum electromagnetics, and classical electromagnetics. Computational electromagnetics can play an important role in Casimir force calculation.**

I. Introduction

In the beginning, electromagnetic analyses, like many science and engineering analyses, were done with pencils and papers. Closed form solutions were sought. However, only limited solutions can be found in closed form. They are restricted to solutions for simple shapes. Later on, approximate solutions were sought for complex shapes. With the advent of computers, computer solutions became important for complex objects. This development not only happens in electromagnetics, but also in other fields in engineering and science, such as computational mechanics, fluid dynamics, and physics. Nowadays, computational electromagnetics replaces pencil and paper analyses: Computational electromagnetics has changed how modern-day scientists and engineers work as electromagnetic simulation tools are used as a virtual laboratory where ideas can be tested, and virtual proto-typing can be performed [1].

Unbeknownst to many, much physical insight of wave and field physics is needed in order to design fast and efficient algorithms for computational electromagnetics; we will discuss some of the pertinent physics involved relevant to the design of fast computational algorithms. For instance, wave field is oscillatory and static field is smooth. This difference has affected the development of fast algorithms for computational electromagnetics: it is a lot easier to accelerate static field calculation, but very difficult to develop fast algorithms for wave physics problems [2].

While wave physics is important in electromagnetics, it is also important in many modern physical concepts such as mesoscopic physics [3], coherence and decoherence in quantum systems [4], and Casimir force calculation [5][5][7]. When the dimensions of electronic devices are on the order of the mean free path of the electrons, wave physics and interference phenomena are important in describing the behavior of electrons in these mesoscopic scale devices. For instance, the concept of coherence is important in optics in the electromagnetic spectrum because of the short wavelength at optical frequencies [8]. Due to the high momentum of electrons, the electronic wavelength is much smaller than optical wavelength. This makes the coherence length of electrons to be much smaller than those in optics. As a result, a quantum system becomes decoherent when coupled to random phenomena or structures. Since a quantum system can never be isolated, and the coupling of one quantum system to another rapidly decoheres a quantum state. Hence, the design of quantum computers is extremely difficult [8][9][10].

Lastly, the meaning of nothingness does not exist in quantum electromagnetics, because there is fluctuating electromagnetic field even in vacuum where classical electromagnetics implies zero field. The vacuum fluctuation gives rise to attractive forces between objects that are in close proximity to each other. The calculation of Casimir force requires using combination of computational electromagnetics, statistical physics, and quantum electromagntics.

II. The Physics of Oscillatory and Smooth Kernels

The kernel of our integral equation is the Green's function. Hence, the interaction in electromagnetic field is via the scalar Green's function and its derivatives [11]:

$$G(\mathbf{r},\mathbf{r}')=\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|} \qquad (1)$$

This kernel is oscillatory due to the exponential function in the numerator. When the frequency, $k\rightarrow 0$, the numerator becomes one, and the Green's function becomes:

$$G(\mathbf{r},\mathbf{r}')=\frac{1}{4\pi|\mathbf{r}-\mathbf{r}'|} \qquad (2)$$

The second Green's function is non-oscillatory even though it has a singularity. When $|\mathbf{r}-\mathbf{r}'|$ is not small, the higher order derivatives of (1) become larger with the increasing order of the derivatives and frequency. But the higher order derivatives of (2) become smaller with increasing order. This is indicative of the fact that (2) cannot carry information long distance, while (1) can convey information long distance [2]. As a consequence, electromagnetic wave field can send information long distance such as across the galaxy, while static field cannot do so. This has significant impact on the design of fast electromagnetic algorithms.

In computational electromagnetics, the interaction matrix is the matrix representation of the Green's function. A matrix element of the matrix representation of the Green's function, in Dirac notation, is [12][13]:

$$A_{mn} = \langle m | G | n \rangle \tag{3}$$

In the above, and function $|m\rangle$ or $|n\rangle$ can represent basis functions defined in the spatial domain. They can represent localized functions defined in a finite domain basis. Hence, when the basis functions $|m\rangle$ and $|n\rangle$ are located far apart, their interaction is dominated by the asymptotic behavior of the Green's function. In the case of wave or oscillatory kernel, information is conveyed between the two functions irrespective of their separation distances. But in the case of static or non-oscillatory kernel, the larger the separation, the less information is conveyed between the two interactions, and such matrix elements are unimportant.

Therefore, for static kernels, the matrix equation that results from the Green's function can often be compressed easily. This can be done via wavelets [14][15][16][17][17], fast multipole methods [18][18], or other matrix compression techniques, such as the adaptive cross approximation method [19].

However, for oscillatory kernels, fast algorithm for solving the matrix equation for sparse scatterers did not arise until the multi-level fast algorithm was developed [20][21]. Simple matrix compression method, or wavelets, or even simple fast multipole method did not give rise to a fast method of solving very large systems in computational electromagnetics when wave physics is involved.

III. Impact on Tree-Based Algorithms

Next, we will give a brief description of the tree-based algorithm that is the basis of the fast multipole method and the multi-level fast multipole algorithm. This allows one to perform a fast matrix-vector product with the matrix in (3). In the tree-based algorithm, the Green's function is factorized using the translational-addition theorem.

$$A_{ij} = \mathbf{V}^t_{il_1} \bullet \overline{\boldsymbol{\beta}}_{l_1 l_2} \bullet \overline{\boldsymbol{\beta}}_{l_2 l_3} \cdots \overline{\boldsymbol{\beta}}_{l_{L-1} l_L} \bullet \overline{\boldsymbol{\alpha}}_{ll'} \bullet \overline{\boldsymbol{\beta}}_{l_L l_{L-1}} \cdots \overline{\boldsymbol{\beta}}_{l_3 l_2} \bullet \overline{\boldsymbol{\beta}}_{l_2 l_1} \bullet \mathbf{V}_{l' j} \tag{4}$$

Such factorization allows information transfer from j to i to be performed in a multi-stage manner, to emulate the telephone network so that a tree algorithm can be written to perform the matrix vector product.

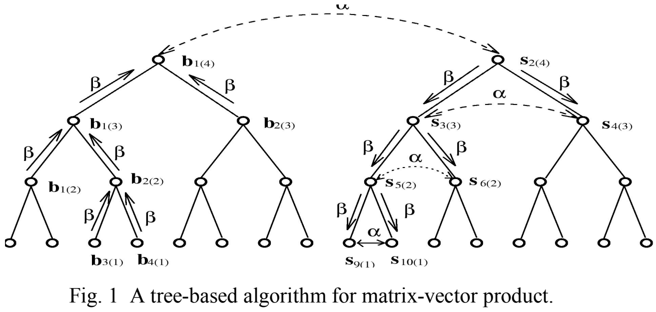

Fig. 1 A tree-based algorithm for matrix-vector product.

In a matrix-vector product, the information from N sources are transmitted to N other sources. This nominally requires N^2 operations for a dense matrix indicated in (3). By using a tree algorithm, the number of communication links can be reduced to $O(N)$ links. If the communication cost for each link is $O(1)$ or of constant cost, then the cost of the matrix vector product is $O(N)$. This in fact happens for static problems as information does not travel long distance for a static kernel. Most of the communication activities are near-neighbor, or happen near the bottom part of the inverted tree in Figure 1.

However, for dynamic or wave problems, the oscillatory kernel transmits information long distance, and hence, the communication is important at all level of the tree. As a result, there is a swelling of information at the top level of the inverted tree, and it is extremely expensive to communicate information near the top of the tree. Hence, a naïve tree algorithm does not result in an algorithm of $O(N \log N)$ complexity. The multi-level fast multipole algorithm uses interpolation and anterpolation [22] to down sample and up sample the data between the levels. Only with this treatment can an $O(N \log N)$ algorithm for matrix-vector product be arrived at.

IV. The Tale of Three Physics

The changing frequency of the kernel causes the physics of the Green's function to change. In fact, it also changes the physics of electromagnetics. At low frequency, or when the wavelength is long compared to the structure that electromagnetic field interacts with, the physics is that of circuit physics. In circuit physics, the electric field and the magnetic field are weakly coupled. This gives rise to two different worlds: the world of the capacitor, and the world of the inductors. These two worlds are weakly coupled, and are decoupled at zero frequency. When the circuit physics is coupled to nonlinear devices like transistors and diodes, its physics is greatly enriched. The successful technologies of micro-electronics and nano-electronics are testimonials of this richness. Peering into the microscopic world of electronics is like Alice in Wonderland.

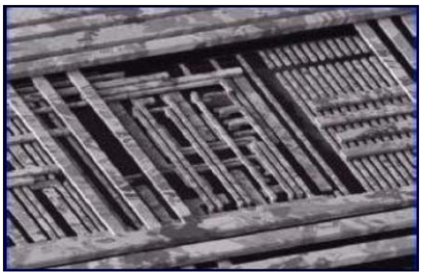

Fig. 2 Peering into the world of microelectronics is like Alice in Wonderland where rich physics exists, and circuit theory applies (courtesy of Intel).

As the frequency becomes higher, such that the structure size is about the wavelength, the coupling between electric field and magnetic field through space becomes stronger; they cannot be considered independent of each other. This is the realm of electromagnetic waves. The wave nature occurs in a physical system when there is an exchange of two kinds of stored energies. In the case of electromagnetics, these are stored electric and magnetic energies. In a mechanical system, it can be potential and kinetic energies.

In this regime, one has often to solve partial differential equations such as Maxwell's equations, Navier-Stokes equations, or equation of elasticity to capture the physics of the wave [23].

Fig. 3 Wave phenomenon as observed in nature.

As the frequency gets higher, waves start to behave like rays, and much of their physics can be captured by ray optics. In ray optics, electromagnetic field is deflected and reflected like particles [24].

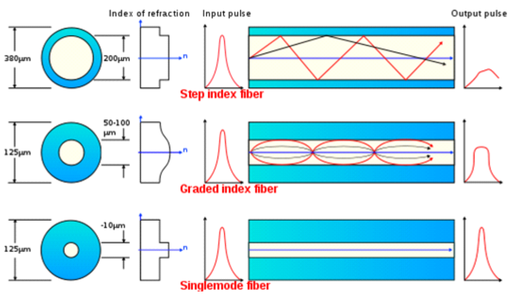

Fig. 4 Travelling of light in optical fiber can be easily understood by ray tracing, which treats light as particles (courtesy of Wiki).

Wave carries a phase when it propagates. When the wavelength is very short, this phase is rapidly varying over space. Hence, one needs to introduce the concept of optical coherence over space and time [8]. When more than one ray propagate in space, they could interfere constructively or destructively with respect to each other. When the two waves are not in phase, they are incoherent, and hence, will interfere destructively.

Moreover, when two fields add, the rapid phase variation and incoherence cause the cross term to average to zero:

$$\begin{aligned}\left\langle |\mathbf{E}_1+\mathbf{E}_2|^2\right\rangle &= \left\langle |\mathbf{E}_1|^2\right\rangle + \left\langle |\mathbf{E}_2|^2\right\rangle + 2\,\mathrm{Re}\left\langle \{\mathbf{E}_1\bullet\mathbf{E}_2^*\}\right\rangle \\ &= \left\langle |\mathbf{E}_1|^2\right\rangle + \left\langle |\mathbf{E}_2|^2\right\rangle\end{aligned} \tag{5}$$

Hence, the addition of energy is like the addition of energy of particles. This has been the basis for radiative transfer theory used in remote sensing and astronomy [25].

V. Quantum Physics

While wave physics is often observed in classical physics pheonomena as in classical electromagentics, it is also prevalent in modern physics such as quantum physics [26]. Particles in quantum mechanics are described by the Schrodinger wave equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},t)+V(\mathbf{r})\psi(\mathbf{r},t)=i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) \tag{6}$$

For vacuum ($V=0$), an admissible solution to the above equation is

$$\psi(\mathbf{r},t)=Ae^{i\mathbf{k}\cdot\mathbf{r}-i\omega t} \tag{7}$$

which describes the wave function of a particle with momentum $\mathbf{p}=\hbar\mathbf{k}$, and kinetic energy $E=\hbar^2|\mathbf{k}|^2/(2m)$. In order to satisfy (6), we also require that $E=\hbar\omega$. The above wave function describes a particle that is equally likely to be found everywhere. This is irrespective of the mass of the particle, and the above remains an admissible solution of (6).

However, when the mass of the particle is large, we expect classical physics to prevail. So when the particle is massive, its momentum is large, and the corresponding k is large. Equation (7) then describes a rapidly varying wave function indicating that the particle is likely to be found everywhere, vastly different from classical physics. But a quantum system is never truly isolated. For instance, it will be connected to other heat baths in the universe. Therefore, (6) alone describes an isolated quantum system which is not realistic. When (6) is coupled to other quantum systems, like heat baths, (7) is highly unstable as a solution, as the phase relationship between the particle at two positions is random. In this case, the particle wave function is better described by a linear superposition of wave packets at different locations where the phase relation between the wave packets is incoherent. When this is expressed in terms of density matrix, the off-diagonal elements of the matrix are zero [26]. This concept is also very important in quantum optics [27][28].

When electrons move about in an environment in which the wavelength of its accompanying Schrodinger wave is small compared to the scatterers (impurity) in the system, the electron wave behaves like rays, and hence, electron behaves like a classical particle in this limit. However, when electronic devices become small, such that the size of the scatterers is comparable to wavelength, the wave nature of the electron wave function becomes important. This is the regime of mesoscopic physics where quantum transport becomes important [3]. Much understanding of wave physics in classical physics can help with the understanding of electronic transport in this regime. When the size of the scatterer is much smaller than the wavelength, then the true wave nature of the Schrodinger wave becomes important.

This is the case of electron wave inside an atom, or around an atom.

VI. Casimir Force

An area that strings classical electromagnetics, statistical physics and quantum electrodynamics nicely together is the area of Casimir force calculation. Casimir force causes two objects to be attracted to each other due to the vacuum fluctuation of electromagnetic field in between the two objects. This attraction occurs even at zero temperature and that the electromagnetic field is in the ground quantum state. Classically, this corresponds to a zero field in between the object, but quantum mechanically, the ground state field produces a force on the object. This force is important of designing micro- and nano-electro-mechanical systems.

Statistical physics states that electromagnetic energy will be created in any vacuum that is in thermal equilibrium with a heat bath. According to the fluctuation dissipation theorem, the electromagnetic energy generated is given by the formula [6]:

$$\left\langle 0\left|\hat{E}_i(\mathbf{r},t)\hat{E}_k(\mathbf{r},t)\right|0\right\rangle = -i\frac{\hbar}{\pi}\int_0^\infty d\omega\omega^2 \operatorname{Im}\{G_{ik}(\mathbf{r},\mathbf{r},\omega\}\coth\frac{\hbar\omega}{2T} \quad (8)$$

In the above, $\hat{E}_k(\mathbf{r},t)$ is the quantum field operator for the electric field, G_{ik} is the dyadic Green's function for the complex geometry, and T is the temperature. The dyadic Green's function for complex geometry can be found using classical computational electromagnetics technique. Hence, computational electromagnetics is important in Casimir force calculation.

VII. Conclusions

Computational electromagnetic is a field that involves the use of mathematics and physical insight to arrive at useful and efficient algorithms. In order to design good computational electromagnetics algorithms, one needs to understand well the physics of the field and wave involved. It is much easier to design fast algorithms for long wavelength interaction, but much harder to arrive at one for short wavelength physics.

Electromagnetic wave physics permeates many of our everyday phenomena, but wave physics is also found in quantum waves for electronic and atomic transport. The understanding of wave physics in the classical level allows us to understand the mesoscopic and microscopic transport in electronic systems.

An area that strings together multi-physics phenomena is the calculation of Casimir force in objects with microscopic separation. The quantum fluctuation of electromagnetic field gives rise to a force that causes stiction in micro- and nano-electro-mechanical systems. It is also a multi-physics calculation that combines the interest of many different areas of physics and between electrical and mechanical engineering.

References

[1] W. C. Chew, J. M. Jin, E. Michielssen, and J. M. Song, (editors), *Fast and Efficient Algorithms in Computational Electromagnetics,* Artech House, Boston, MA, 2001.

[2] W. C. Chew, "Computational Electromagnetics---the Physics of Smooth versus Oscillatory Fields," *Philo. Trans. Royal Soc. London Series A, Math., Phys. Eng. Sci.* vol. 362, no. 1816, pp. 579-602, March 15, 2004.

[3] S. Datta, *Electronic Transport in Mesoscopic Systems*, Cambridge University Press, Cambridge, 1995.

[4] W. H. Zurek: *Decoherence and the Transition from Quantum to Classical—Revisited,* Los Alamos Science Number 27 2002.

[5] H. B. Chan, V. A. Aksyuk, R. N. Kleinman, D. J. Bishop, and F. Capasso, "Quantum mechanical actuation of microelectromechanical systems by the Casimir force," *Science* 291, pp. 1941-1944, 2001.

[6] A. Rodriguez, M. Ibanescu, D. Iannuzzi, J. D. Joannopoulos, and S.G. Johnson, "Virtual photons in imaginary time: Computing exact Casimir forces via standard numerical electromagnetism techniques**,"** *Phys. Review* A., vol. 76, p 032106, 2007.

[7] J. L. Xiong, W. C. Chew, "Efficient Evaluation of Casimir Force in 2.5D Problems by Integral Equation Methods", Applied Physics. Letter, vol. 95, 154102, Oct. 2009.

[8] L. Mandel and E. Wolf, "Coherence properties of optical fields," *Rev. Mod. Phys.*, 37:23187, 1965.

[9] D. P. DiVincenzo, "Quantum Computation". *Science* **270** (5234): 255–261, 1995.

[10] M.A. Nielsen and I.L. Chuang. *Quantum Computation and Quantum Information,* New York, NY: Cambridge University Press, 2000.

[11] J.A. Kong, *Theory of Electromagnetic Waves*, Wiley-Interscience, New York, 1975.

[12] R.F Harrington**,** Field Computation by Moment Methods, MacMillan, New York, 1968.

[13] S.M. Rao, D.R. Wilton, and A.W. Glisson, Electromagnetic scattering by surfaces of arbitrary shape, *IEEE Trans Antennas Propagat* AP-30, 409-418, 1982.

[14] B. A Alpert, G. Beylkin, R.R. Coifman, and V. Rokhlin, "Wavelet-like bases for the fast solution of second-kind integral equations," *SIAM J. Sci. Comput*., vol. 14, no. 1, pp. 159--184, 1993.

[15] H. Kim and H. Ling, "On the application of fast wavelet transform to the integral-equation solution of electromagnetic scattering problems," *Micro. Opt. Tech. Lett*., vol. 6, no. 3, pp. 168--173, 1993.

[16] W. L. Golik, "Sparsity and conditioning of impedance matrices obtained with semi-orthogonal and bi-orthogonal wavelet bases," *IEEE Trans. Ant. Propag*., vol. 48, no. 4, pp. 473--481, 2000.

[17] R.L. Wagner and W.C. Chew, "A study of wavelets for the solution of electromagnetic integral equations," *IEEE Trans. Ant. Propag*., vol. 43, no. 8, pp. 802--810, 1995.

[18] L. Greengard and V. Rokhlin, "A Fast Algorithm for Particle Simulations," *J. Comp. Phys.*, vol. 73, pp. 325--348, 1987.

[19] M. Bebendorf, "Approximation of boundary element matrices," Numer. Math., 86: 565–589, 2000.

[20] C.C. Lu and W.C. Chew, "A multilevel algorithm for solving a boundary integral equation of wave scattering," *Micro. Opt. Tech. Lett*., vol. 7, no. 10, pp. 466-470, July 1994.

[21] J.M. Song and W.C. Chew, "Multilevel fast-multipole algorithm for solving combined field integral equations of electromagnetic scattering," *Mico. Opt. Tech. Lett*., vol. 10, no. 1, pp 14-19, Sept. 1995.

[22] A. Brandt, "Multilevel computations of integral transforms and particle interactions with oscillatory kernels," *Comp. Phys. Comm*., vol. 65, pp. 24-38, 1991.

[23] W.C. Chew, M. S. Tong, and B. Hu, *Integral Equations Methods for Electromagnetic and Elastic Waves*, Morgan & Claypool, 2008.

[24] J.B. Keller, "Geometrical theory of diffraction," *J. Opt. Soc. Amer*., 52, pp. 116-130, 1962.

[25] S. Chandrasekhar, *Radiative Transfer*, New York: Dover, 1960.

[26] E. Merzbacher, *Quantum Mechanics*, Wiley, John & Sons, 1998.

[27] C. C. Gerry and P. L. Knight, *Introductory Quantum Optics*, New York, NY: Cambridge University Press, 2004.

[28] H.P. Yuen and J.H. Shapiro. "Optical Communication with Two-Photon Coherent States-Part III: Quantum Measurements Realizable with Photoemissive Detectors." *IEEE Transactions on Information Theory* IT-26: 78-92, 1980.